

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.76e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.09e-01

Confidence level: 3.25e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Lenacil</div> <div>Measured: 2.56e-05</div> <div>Predicted: 1.78e-04</div>	<div>Image not found</div> <div>Amidithion</div> <div>Measured: 7.32e-02</div> <div>Predicted: 5.25e-02</div>	<div>Image not found</div> <div>Ethoate-methyl</div> <div>Measured: 3.49e-02</div> <div>Predicted: 5.28e-02</div>
<div>Image not found</div> <div>Endosulfan</div> <div>Measured: 1.14e-06</div> <div>Predicted: 6.37e-06</div>	<div>Image not found</div> <div>Endosulfan I</div> <div>Measured: 1.14e-06</div> <div>Predicted: 6.37e-06</div>	<div>Image not found</div> <div>Endosulfan II</div> <div>Measured: 1.14e-06</div> <div>Predicted: 6.37e-06</div>
<div>Image not found</div> <div>Tranid</div> <div>Measured: 8.28e-03</div> <div>Predicted: 1.40e-02</div>		

